

di-(2-Methoxybutyl)oxalate

Inchi:	InChI=1S/C12H22O6/c1-5-9(15-3)7-17-11(13)12(14)18-8-10(6-2)16-4/h9-10H,5-8H2,1-4
InchiKey:	GPABTUKRFXERRO-UHFFFAOYSA-N
Formula:	C12H22O6
SMILES:	CCC(COC(=O)C(=O)OCC(CC)OC)OC
Mol. weight [g/mol]:	262.30

Physical Properties

Property code	Value	Unit	Source
gf	-632.56	kJ/mol	Joback Method
hf	-1055.61	kJ/mol	Joback Method
hfus	27.74	kJ/mol	Joback Method
hvap	64.66	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.923		Crippen Method
mcvol	206.560	ml/mol	McGowan Method
pc	1896.95	kPa	Joback Method
rinsol	1327.00		NIST Webbook
tb	670.50	K	Joback Method
tc	852.67	K	Joback Method
tf	383.78	K	Joback Method
vc	0.779	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.78	J/molxK	670.50	Joback Method
cpg	586.51	J/molxK	700.86	Joback Method
cpg	600.54	J/molxK	731.22	Joback Method
cpg	613.86	J/molxK	761.58	Joback Method
cpg	626.44	J/molxK	791.94	Joback Method
cpg	638.28	J/molxK	822.31	Joback Method
cpg	649.34	J/molxK	852.67	Joback Method
dvisc	0.0012699	Paxs	383.78	Joback Method
dvisc	0.0006179	Paxs	431.57	Joback Method

dvisc	0.0003471	Paxs	479.35	Joback Method
dvisc	0.0002165	Paxs	527.14	Joback Method
dvisc	0.0001460	Paxs	574.93	Joback Method
dvisc	0.0001046	Paxs	622.71	Joback Method
dvisc	0.0000786	Paxs	670.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R542159&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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